

## ADVANCES IN THE THEORY OF BOX INTEGRALS

D. H. BAILEY, J. M. BORWEIN, AND R. E. CRANDALL

**ABSTRACT.** Box integrals—expectations  $\langle |\vec{r}|^s \rangle$  or  $\langle |\vec{r} - \vec{q}|^s \rangle$  over the unit  $n$ -cube—have over three decades been occasionally given closed forms for isolated  $n, s$ . By employing experimental mathematics together with a new, global analytic strategy, we prove that for each of  $n = 1, 2, 3, 4$  dimensions the box integrals are for any integer  $s$  hypergeometrically closed (“hyperclosed”) in an explicit sense we clarify herein. For  $n = 5$  dimensions, such a complete hyperclosure proof is blocked by a single, unresolved integral we call  $\mathcal{K}_5$ ; although we do prove that all but a finite set of  $(n = 5)$  cases enjoy hyperclosure. We supply a compendium of exemplary closed forms that arise naturally from the theory.

### 1. PRELIMINARIES

We define *box integrals*<sup>1</sup> for positive-integer dimension  $n$  as expectations of  $|\vec{r}|^s$ ,  $|\vec{r} - \vec{q}|^s$  with the relevant vectors chosen randomly, independently, equidistributed over the unit  $n$ -cube<sup>2</sup> [13]:

$$\begin{aligned} B_n(s) &:= \int_{\vec{r} \in [0,1]^n} |\vec{r}|^s \mathcal{D}\vec{r} \\ (1) \quad &= \int_0^1 \cdots \int_0^1 (r_1^2 + \cdots + r_n^2)^{s/2} dr_1 \cdots dr_n, \\ \Delta_n(s) &:= \int_{\vec{r}, \vec{q} \in [0,1]^n} |\vec{r} - \vec{q}|^s \mathcal{D}\vec{r} \mathcal{D}\vec{q} \\ (2) \quad &= \int_0^1 \cdots \int_0^1 ((r_1 - q_1)^2 + \cdots + (r_n - q_n)^2)^{s/2} dr_1 \cdots dr_n dq_1 \cdots dq_n. \end{aligned}$$

Here,  $\mathcal{D}\vec{r}$  denotes simply the volume element  $dr_1 dr_2 \cdots$ . As explained in a previous treatment [5], there are physical interpretations:

- (1)  $B_n(1)$  is the expected distance of a random point from the origin (or from any fixed vertex) of the  $n$ -cube;
- (2)  $\Delta_n(1)$  is the expected distance *between* two random points of the  $n$ -cube;

Received by the editor March 3, 2009 and, in revised form, August 13, 2009.

2010 *Mathematics Subject Classification.* Primary 11Y60; Secondary 28-04.

The first author was supported in part by the Director, Office of Computational and Technology Research, Division of Mathematical, Information, and Computational Sciences of the U.S. Department of Energy, under contract number DE-AC02-05CH11231.

The second author was supported in part by ARC, NSERC and the Canada Research Chair Programme.

<sup>1</sup>Not to be confused with “box integrals” of particle physics.

<sup>2</sup>We refer to “box integrals” but use the term “ $n$ -cube” for the domain hypercube.

- (3)  $B_n(-n+2)$  is the expected electrostatic potential in an  $n$ -cube whose origin has a unit charge;<sup>3</sup>
- (4)  $\Delta_n(-n+2)$  is the expected electrostatic energy between two points in a uniform cube of charged “jellium”.

Note that the definitions show immediately that both  $\Delta_n(2m)$  and  $B_n(2m)$  are rational when  $m, n$  are natural numbers. A pivotal, original treatment on box integrals is the 1976 work of Anderssen et al. [1]. There have been interesting modern treatments of the  $B_n$  and related integrals, as in [7], [11, p. 208], [27] and [25]. Related material is also to be found in [16, 26].

There are other similar entities such as the expected distance between points on distinct sides of a cube or hypercube investigated in [11, §1.7] and [7]. We remark that  $B_3(1)$  is also known as the Robbins constant, after [22].

It is worth noting that the methods of the present paper actually have practical application—for example in biology, of all places. In the work [14] these new box-integral evaluations are being used as one measure of “how random?” is a point cloud. That is, one test of whether brain synapses are sufficiently randomly distributed involves comparison of empirical values  $\langle |\vec{r} - \vec{q}|^s \rangle$ , where  $\vec{r}, \vec{q}$  run over synapse positions, against our present theoretical tabulations of  $\Delta_3(s)$ .

## 2. QUADRATURE FORMULAE FOR ALL COMPLEX POWERS

As in our previous treatment [5], we define two key functions as

$$(3) \quad b(u) := \int_0^1 e^{-u^2 x^2} dx = \frac{\sqrt{\pi} \operatorname{erf}(u)}{2u},$$

$$(4) \quad d(u) := \int_0^1 \int_0^1 e^{-u^2(x-y)^2} dx dy = \frac{-1 + e^{-u^2} + \sqrt{\pi} u \operatorname{erf}(u)}{u^2}.$$

These functions may be used as integration kernels, in the following way. Writing

$$(5) \quad R^s = \frac{1}{\Gamma(-s/2)} \int_0^\infty t^{-s/2-1} e^{-tR^2} dt,$$

as valid for  $\Re(s) < 0$ , we can integrate formally over  $R$  (being a radius, or a separation) in a relevant region, to obtain

$$(6) \quad B_n(s) = \frac{2}{\Gamma(-s/2)} \int_0^\infty u^{-s-1} b^n(u) du,$$

$$(7) \quad \Delta_n(s) = \frac{2}{\Gamma(-s/2)} \int_0^\infty u^{-s-1} d^n(u) du;$$

both representations being valid for a *reduced* range of complex  $s$ , namely the range  $\Re(s) \in (-n, 0)$ . This domain of convergence for the integrals can be inferred from the large- $u$  asymptotic behaviors; see e.g., [2],

$$(8) \quad b(u) = \frac{1}{u} + O\left(e^{-u^2}\right),$$

$$(9) \quad d(u) \sim \frac{\sqrt{\pi}}{u} - \frac{1}{u^2} + O\left(e^{-u^2}\right),$$

so that having integrand factors  $b^n, d^n$ , respectively, allows integral convergence for the stated range  $\Re(s) \in (-n, 0)$ . Throughout,  $n$  will denote a natural number.

<sup>3</sup>Such statements presume that electrostatic potential in  $n$  dimensions is  $V(r) = 1/r^{n-2}$ , and say  $\log r$  for  $n = 2$ ; the main issue being that negative powers of  $r$  can also have physical meaning.

What can we say about analytic continuation in  $s$ ? We can extend such previous results to *all* complex  $s$ , by paying closer attention to integrand structure. First, we can extend the region for negative  $\Re(s)$  arbitrarily, by finding superpositions of terms  $b(ku)$  or  $d(ku)$ , for integers  $k$ , such that the  $n$ -th powers of the asymptotic forms (8), (9) are genuinely of exponential decay.

Second, for positive  $\Re(s)$  and a positive integer  $K$ , we may employ the integral identity

$$(10) \quad D(\rho, K) := \int_0^\infty t^{-\rho-1} (1 - e^{-tu})^K du = \Gamma(-\rho) \sum_{j=1}^K \binom{K}{j} (-1)^j j^\rho$$

from which it is straightforward to derive integral representations for all  $s$  in the open right half-plane except for the positive even integers.

**Theorem 1** (Quadrature formulae for general complex  $s$ ). *In the region with  $\Re(s) < 0$  we have*

$$(11) \quad B_n(s) = \frac{2}{1 - 2^{n+s}} \frac{1}{\Gamma(-s/2)} \int_0^\infty u^{-s-1} (b^n(u) - 2^n b^n(2u)) du.$$

For  $\Delta_n(s)$  in the same  $s$ -region, let  $A_1 := 1$  and consider the unique solution  $(A_2, \dots, A_{n+2})$  to the linear system

$$(12) \quad 0 = \sum_{k=1}^{n+2} \frac{A_k}{k^q}, \quad q = 0, 1, 2, \dots, n.$$

Then

$$(13) \quad \Delta_n(s) = \frac{2}{\Gamma(-s/2)} \left( \sum_{k=1}^{n+2} A_k k^{n+s} \right)^{-1} \int_0^\infty u^{-s-1} \left( \sum_{k=1}^{n+2} A_k k^n d^n(ku) \right) du.$$

Next, consider the region  $\Re(s) \in (0, 2K)$  with  $K$  a positive integer and  $s$  not an even integer. We have

$$(14) \quad B_n(s) = \frac{2}{D(s/2, K)} \int_0^\infty u^{-s-1} du \sum_{j=1}^K \binom{K}{j} (-1)^j b^n(u\sqrt{j}),$$

$$(15) \quad \Delta_n(s) = \frac{2}{D(s/2, K)} \int_0^\infty u^{-s-1} du \sum_{j=1}^K \binom{K}{j} (-1)^j d^n(u\sqrt{j}).$$

*Remark.* As for nonnegative even integers  $s$  not covered in the above theorem, the definitions (1), (2) immediately yield rational values for  $B_n, D_n$ , respectively, upon symbolic integration.

It is interesting that even though the goal of the above development is to provide practical quadrature formulae, we already have a byproduct:

**Corollary 1** (Pole structure of the box integrals).  $B_n(s)$ , for positive integer  $n$ , has precisely one pole, namely at  $s = -n$ .  $\Delta_n(s)$ , on the other hand, always has precisely  $(n+1)$  poles, located at  $s = -2n, -2n+1, \dots, -n$ .

*Proof.* Clearly, by the original definitions (1) and (2),  $B_n(s), \Delta_n(s)$  are both finite for nonnegative  $\Re(s)$ , so it suffices to look at negative  $\Re(s)$  in any case. For  $B_n(s)$ , relation (11) has a pole factor at  $s = -n$ .

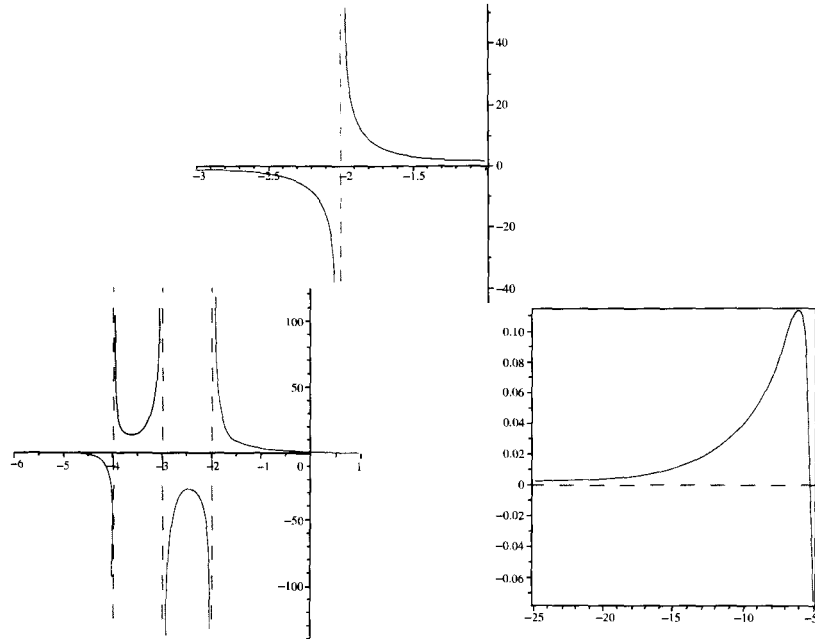


FIGURE 1. Analytic continuation: Plots of  $B_2(s)$  (top) and  $\Delta_2(s)$  (bottom) for real  $s$  in various intervals.  $B_2(s)$  is the expected value of  $r^s$  where  $r$  is the distance from origin to a random point on the unit square  $[0, 1]^2$ . Likewise,  $\Delta_2(s)$  is the expectation with  $r$  being the distance between two random points.  $B_2(s)$  has a solitary pole at  $s = -2$ , while  $\Delta(s)$  has three poles at  $s = -2, -3, -4$ . Evidently,  $\Delta_2(s)$  also has a mysterious zero at some real  $s \approx -5.137 \dots$  (see text).

As for  $\Delta_n(s)$ , the solution  $(A_k)$  to the system of equations is unique since the matrix with entries  $(-1)^k/(k+1)^{j-1}$  for  $1 \leq k, j \leq n$  is nonsingular with determinant  $(-1)^{\lfloor n/2 \rfloor} \prod_{i=1}^{n-1} \frac{i!}{(n+1)!}$  (see sequence A002109 in Sloane's *Online Encyclopedia of Integer Sequences*). Poles of  $\Delta_n$  force the prefactor  $\sum_{k=1}^{n+2} A_k k^{n+s}$  to vanish exactly when  $n+s \in [-n, 0]$ , thus giving a total of  $(n+1)$  poles on the negative real  $s$ -axis. It remains to check that  $\sum_{k=1}^{n+2} A_k k^{n+s}$  has no other zeros. This runs as follows. Consider the more general exponential sum

$$\Phi_N(t) := \sum_{j=1}^N \alpha_j \beta_j^t = 1$$

for arbitrary real constants  $\alpha_j$  and positive  $\beta_j$ . If  $\Phi_N(t) = 1$  has more than  $N$  solutions, then Rolle's theorem and some manipulation will produce a derived system with at least  $N$  solutions and one less term. We are done, since when  $N = 1$  this is impossible.  $\square$

By employing the quadrature options embodied in Theorem 1, we have been able to calculate various  $B_n(s)$ ,  $\Delta_n(s)$  values to extreme precision.<sup>4</sup>

One may also use the quadrature prescription to create contiguous plots of box integrals, as in Figure 1. Referring to Figure 1, note that both plots show the “natural” pole at  $s = -2$ , where the standard expectation integral diverges for  $n = 2$  dimensions. However, we see that  $\Delta_2$  also has poles at  $s = -3, -4$  as in Corollary 1.

### 3. QUADRATURE EXPERIMENTS

We have employed the quadrature schema of Theorem 1 to effect extreme-precision values. We might mention here that in fact this research began in earnest with the discovery, using the PSLQ integer relation algorithm (see [15] and [8]), that the extreme-precision numerical value we were able to compute for  $\Delta_3(-1)$ , namely

$$(16) \quad \Delta_3(-1) = 1.88231264438966016010560083886836758785246288031070\dots$$

was (experimentally) given by the formula

$$(17) \quad \Delta_3(-1) \stackrel{?}{=} \frac{2}{5} + \frac{2}{5}\sqrt{2} - \frac{4}{5}\sqrt{3} - \frac{2}{3}\pi - 6\log 2 + 2\log(1 + \sqrt{2}) \\ + 12\log(1 + \sqrt{3}) - 4\log(2 + \sqrt{3}).$$

Soon we were able to prove this evaluation.<sup>5</sup> Upon further experimentation and analytic discoveries, we realized that not only do some  $B_n$  for various  $n$  have constants in common—such as log-surds,  $\pi$ , and so on—but the  $\Delta_n$  constants also have many constants in common with themselves and the  $B_n$ . Such experimentation/detection moved us to find algebraic relations between the various entities, as we describe in this paper.

Our numerical approach was to implement, using the Fortran-90 interface to the ARPREC arbitrary precision software package [10], the four formulae of Theorem 1, namely (11), (13), (14) and (15), and the definitions of the functions  $b(u)$ ,  $d(u)$  and  $D(\rho, K)$  as given by formulae (4), (3) and (10). As stated in Theorem 1, these formulae are valid for all  $s$  except for positive even integers. For positive even arguments the integration in (1), (2) is trivial and the relevant box integral is rational, obtainable quickly with symbolic processing.<sup>6</sup>

Computation of  $b(u)$  is entirely straightforward, once one has in hand an implementation of the erf function (see [2, pp. 297–298]).

Computation of  $d(u)$  is complicated by the fact that for small arguments, cancellation of terms in the numerator typically results in severe relative numerical error.

<sup>4</sup>As in previous works, by “extreme precision” we mean, loosely speaking, enough precision to resolve a given entity into fundamental (or at least previously studied) constants; in the modern era—the age of, say, LLL and PSLQ methods—this usually means precision to hundreds to thousands of decimal digits.

<sup>5</sup>That is to say, the  $\stackrel{?}{=}$  became  $=$ . In the present work, we use  $=$  to mean rigorously proven; indeed, some of our more recondite closed forms were first found in the  $\stackrel{?}{=}$  sense, then later proven.

<sup>6</sup>*Mathematica* and *Maple* were both used quite heavily for much of this paper’s development, and most of the work was symbolic. We have endeavored to check all results numerically, even after obtaining exact, symbolic forms. That being said, elsewhere in this paper we have for efficiency eschewed comments about which computer algebra system was used where.

This can be ameliorated by employing the Taylor series for  $d(u)$ :

$$(18) \quad d(u) = 1 - \frac{u^2}{6} + \frac{u^4}{30} - \frac{u^6}{168} + \frac{u^8}{1080} - \frac{u^{10}}{7920} + \frac{u^{12}}{65520} - \cdots$$

$$= \sum_{n=0}^{\infty} \frac{(-1)^n u^{2n}}{(2n+1) \cdot (n+1)!}$$

Computation of the  $A_k$  coefficients was achieved by employing an arbitrary precision version of the well-known Linpack program for solving linear equations via LU decomposition [20].

The four formulae (11), (13), (14) and (15) of Theorem 1 themselves involve significant numerical difficulties, as they involve near-cancellation of terms for small arguments. Nonetheless, we were able to compute the  $B_n(s)$  and  $D_n(s)$  to approximately 470-digit accuracy, utilizing 500-digit working precision, by using Gaussian quadrature, after splitting the integral into the intervals  $(0, 1)$  and  $(1, \infty)$ , and applying the simple substitution  $w = 1/u$  on the second integral.

We should add here that tanh-sinh quadrature [24], which we have used in numerous other studies of this sort, was not needed in this case, because each of the integrand functions in Theorem 1 are regular on the intervals of integration. In addition, the tanh-sinh scheme suffers here from the cancellation difficulties mentioned above, since it relies on evaluating the function very close to endpoints of the interval.

The numerical values we obtained in this fashion were used in conjunction with the PSLQ integer relation algorithm to find many of the analytical evaluations presented in this paper. All results are summarized in the Appendix. As explained at the beginning of the Appendix, 400-digit numerical values of these constants are available on a website.

#### 4. VALIDATION OF EXPRESSIONS

To confirm the accuracy of the results in the Appendix, the  $B$  and  $\Delta$  integrals were separately computed using 500-digit working precision, programmed with the C++ interface to the ARPREC package. Integrals were evaluated by formulae (11), (13), (14) and (15), using Gaussian quadrature, and imported into *Mathematica* as numerical values. A parser for LaTeX source provided with *Mathematica* 7.0 was used to import the analytical formulae from the Appendix in a machine-readable format. Conversions were made to use *Mathematica* built-in routines for computing the Lewin arctan integral, Clausen function and hypergeometric function. The accuracy of these formulae was then checked by subtracting the numerical values computed by quadrature with numerical values produced by *Mathematica* for the analytical formulae. In our first application of this method, four errors were found among the  $B_n(s)$  formulae and three among the  $\Delta_n(s)$  given in the Appendix. Fortunately, in all but two cases we were able to find the correct formula merely by running PSLQ on the vector consisting of  $B_n(s)$  or  $\Delta_n(s)$  and the component terms in the flawed identity. These results were then double-checked using *Mathematica*. Diagnosing the errors in the remaining two formulae, assisted also by *Maple 13*, led to significant enhancements in the final version of this paper.

We observe that this type of checking—computing extreme-precision numerical values for specific instances of left-hand side and right-hand side expressions in a formula, then comparing the results—is very generally applicable and highly

effective in disclosing “bugs” in papers presenting new mathematical identities. Its general adoption would prevent many mistakes from making their way into published papers.

### 5. ANALYTIC CONTINUATION FOR THE $B_n$

In our previous work [5] we demonstrated that the  $B_n$  expectations can always be reduced by at least one dimension; for example, via vector-field algebra,  $B_n$  can be obtained from an integral over the  $(n-1)$ -dimensional unit cube, likewise for  $n > 1$ :

$$(19) \quad B_n(s) = \frac{n}{n+s} \int_{\vec{r} \in [0,1]^{n-1}} (1+r^2)^{s/2} \mathcal{D}\vec{r}.$$

Note that *already* with this reduction we see that  $B_n$  has a single, simple pole at  $s = -n$ , as the integral exists for all complex  $s$ .

With the advantage of hindsight, we define right now a general and quite useful function

$$(20) \quad C_{n,k}(s, a) := \int_{\vec{r} \in [0,1]^n} r_1 r_2 \cdots r_k (a + r^2)^{s/2} \mathcal{D}\vec{r},$$

and we also define  $C_{0,0}(s, a) := a^{s/2}$ . In this way we can begin developing relations for the  $B_n$ , as follows:

$$(21) \quad B_1(s) = \frac{1}{s+1} C_{0,0}(s, 1) = \frac{1}{s+1},$$

$$(22) \quad B_2(s) = \frac{2}{2+s} C_{1,0}(s, 1) = \frac{2}{2+s} {}_2F_1\left(\frac{1}{2}, -\frac{s}{2}; \frac{3}{2}; -1\right),$$

$$(23) \quad B_3(s) = \frac{3}{3+s} C_{2,0}(s, 1) = \frac{6}{(3+s)(2+s)} \int_0^{\pi/4} \left( (1 + \sec^2 t)^{s/2+1} - 1 \right) dt.$$

Note that the apparent pole at  $s = -2$  for  $B_3(s)$  is specious; the  $1/(s+2)$  factor cancels in this case, to yield

$$(24) \quad B_3(-2) = 3 \int_0^{\pi/4} \log(1 + \sec^2 t) dt.$$

For  $n = 4$  and higher dimensions, such relations for the  $B_n$  rapidly become unwieldy. Take  $n = 4$ , and note that  $C_3(s, 1)$  is a 3-dimensional integral which yields, after integrating first in polar coordinates  $(r, \phi)$  to handle two of the dimensions,

$$(25) \quad \begin{aligned} B_4(s) &= \frac{4}{4+s} C_{3,0}(s, 1) \\ &= \frac{8}{(4+s)(2+s)} \int_0^{\pi/4} d\phi \int_0^1 \left( (1 + \sec^2 \phi + z^2)^{s/2+1} - (1+z^2)^{s/2+1} \right) dz. \end{aligned}$$

Again, the specious pole factor for  $s = -2$  cancels, giving the special case

$$(26) \quad B_4(-2) = 2 \int_0^{\pi/4} d\phi \int_0^1 (\log(1 + \sec^2 \phi + z^2) - \log(1 + z^2)) dz.$$

There is another form of analytic relation also derived previously [5], namely

$$(27) \quad B_n(s) = \frac{n^{1+s/2}}{n+s} \sum_{k \geq 0} (-s/2)_k \left(\frac{2}{n}\right)^k \beta_{n-1,k},$$

where the  $\beta$  coefficients arise from the  $b$  function, implicitly as

$$(28) \quad \left(b(u)e^{u^2}\right)^n =: \sum_{k \geq 0} \beta_{n,k} 2^k u^{2k},$$

and  $(a)_k = \Gamma(a+k)/\Gamma(a)$  is the Pochhammer symbol.

The  $\beta$  numbers enjoy the relations (here,  $d!!$  means  $1 \cdot 3 \cdots d$  for odd-positive integer  $d$ ):

$$\begin{aligned} \beta_{n,k} &= \sum_{k_1 + \cdots + k_n = k} \frac{1}{(2k_1+1)!!} \cdots \frac{1}{(2k_n+1)!!}, \\ \beta_{n,k} &= \sum_{j=0}^k \frac{1}{(2k+1)!!} \beta_{n-1,k-j}, \\ (29) \quad (1+2k/n) \beta_{n,k} &= \beta_{n,k-1} + \beta_{n-1,k}, \end{aligned}$$

with the recursions here ignited by  $\beta_{0,k} := \delta_{0,k}$  and  $\beta_{n,1} = n/3$ .

The main point is, for  $n > 1$  the sum (27) is *linearly absolutely convergent* for all complex  $s$ . (The summand decay factor is essentially  $(1 - 1/n)^k$ .) Accordingly, the series gives the analytic continuation over the entire  $s$ -plane. This series representation can be used computationally, either in place of the quadrature formulae, or as an extreme-precision check on the same. The analytic series does have one advantage over the quadrature formalism: One need not break the plane by polarity of  $\Re(s)$ ; the series (27) always converges (and there is the correct single-pole factor  $1/(n+s)$ ).

## 6. THEORY OF HYPERCLOSURE

We have seen that the box integrals  $B_n$  are expressible in terms of  $C$ -functions. It will turn out that there exist recurrence relations between  $C$ -functions; this leads eventually to relations between  $\Delta_n$  and  $B_n$  values, and closed forms in many cases.

To quantify for our purposes what is a closed form, we first establish<sup>7</sup>

**Definition 1** (Ring of hyperclosure). We define a *hypergeometric evaluation* in a classical sense –to be a complex number  $\sum_{n \geq 0} a_n z^n$  where  $z$  is complex algebraic,  $a_0$  is a real rational, and generally  $a_{n+1} = r(n) a_n$  where  $r$  is a fixed rational-polynomial function (ratio of two polynomials each with integer coefficients). We then contemplate the *ring of hyperclosure*, generated by all hypergeometric evaluations under ordinary operators  $(\cdot, +)$ . An element of this ring is said to be hypergeometrically closed (*hyperclosed* for short). We also deem  $\infty$  to be hyperclosed (so that hyperclosure cannot be denied at poles).

<sup>7</sup>It has occurred to the present authors that the age-old notion of “closed form” might be addressable, as a separate research program, such as our Definition 1. However, in no sense can Definition 1 be all-encompassing; e.g., most would say that something like  $1/(\pi + e)$  is a “closed form”, yet for all we know it might not lie in our hyperclosure ring.



As examples, any rational (a sum with one term, say  $r := 0$ ) is hyperclosed, and since

$$\sqrt{2} = {}_2F_1\left(-\frac{1}{2}, 1, 1; -1\right), \quad \pi = 4 {}_2F_1\left(\frac{1}{2}, 1, 3/2, -1\right), \quad \log(1+z) = z {}_2F_1(1, 1, 2; -z),$$

it follows that combinations such as  $\sqrt{2} + \pi$ ,  $\pi\sqrt{2}$ ,  $\pi^{10} \log^7 2$ ,  $\frac{1}{3} \log(1 + \sqrt{2})$  are all hyperclosed. Relevant to the present work is the fact that the Lerch transcendent

$$(30) \quad \Phi(z, s, a) := \sum_{n \geq 0} \frac{z^n}{(n+a)^s},$$

is hyperclosed for algebraic  $z$ , integer  $s$ , and rational  $a$ . Thus, we shall have hyperclosure for any polylogarithm  $\text{Li}_s(z) := \sum_{n \geq 1} z^n/n^s$  for integer  $s$  and algebraic  $z$ , so perforce for the Lewin arctan integral

$$(31) \quad \text{Ti}_2(z) := \sum_{n \geq 0} (-1)^n \frac{z^{2n+1}}{(2n+1)^2} = \frac{z}{4} \Phi\left(-z^2, 2, \frac{1}{2}\right),$$

and the Clausen function

$$(32) \quad \text{Cl}_2(z) := \sum_{n \geq 1} \frac{\sin(nz)}{n^2}.$$

Our box-integral tables have hyperclosed entries, except where “dangling integrals” remain when dimension  $n > 4$ . (Although we admit such unresolved integrals may still belong to the ring.)

An interesting sidelight looms here: What numbers are *not* hyperclosed? Certainly we need such numbers to exist, lest our entire research program of finding hyperclosed expressions be a vacuous exercise. Given the algebraic character of parameter  $z$  in Definition 1, and the constraint that the succession ratio  $r(n)$  be rational-polynomial, together with the fact of all group generations under  $(\cdot, +)$  yielding finite strings, we conclude that the ring of hyperclosure is countably infinite. Therefore: *Almost all complex numbers are not hyperclosed.* Equivalently, the ring of hyperclosure is a null set in the complex plane. As often happens in such analyses, we are stultified by the question: “If non-hyperclosed numbers are so overwhelmingly abundant, what is an example of such a number?” Well, we do not presently know a single such number. Perhaps  $\pi^\pi$  is not hyperclosed, but such questions loom Hilbertian in their evident profundity.<sup>8</sup>

It is evident that the lowest-lying  $C$ -functions allow direct hypergeometric evaluation, so that  $B_1(s)$ ,  $B_2(s)$  are hyperclosed for any integer  $s$ , but that already for  $C_{2,0}$  we run into some difficulty with the integration. Happily, there are some powerful connection formulae that we prove presently, starting with

**Theorem 2** (Convergent series for  $C$ -functions). *For all complex  $s$ , integer  $n > 1$ , and  $\Re(a) > 0$  we have*

$$(33) \quad C_{n,0}(s, a) = (n+a)^{s/2} \sum_{k \geq 0} \left(\frac{2}{n+a}\right)^k (-s/2)_k \beta_{n,k},$$

*with expansion being linearly convergent with  $k$ -th summands being  $O(((n-1)/(n+a))^k)$ .*

<sup>8</sup>Such a radical disconnect between theory and knowledge occurs elsewhere; e.g., in the study of normal numbers. Though almost all real numbers are (absolutely) normal, only artificially constructed normals are known.

*Proof.* This expansion can be established using the same methods as for expansion (27), which is the case  $a = 1$  as shown in [5].  $\square$

And now for some key recurrences:

**Theorem 3** (Fundamental relations for  $C$ -functions). *Special instances of the  $C$ -function are*

$$(34) \quad C_{n,0}(s, 0) = B_n(s),$$

$$(35) \quad C_{0,0}(s, a) := a^{s/2},$$

$$(36) \quad C_{n,0}(s, 1) = \frac{n+s+1}{n+1} B_{n+1}(s).$$

More generally, for all complex  $s$ , positive integer  $n$ , and positive real  $a$  we have

$$(37) \quad asC_{n,0}(s-2, a) = (s+n)C_{n,0}(s, a) - nC_{n-1,0}(s, a+1).$$

Another recurrence, now involving the second index on  $C$ , is, for positive integers  $a, k$ ,

$$(38) \quad sC_{n,k}(s-2, a) = C_{n-1,k-1}(s, a+1) - C_{n-1,k-1}(s, a).$$

*Proof.* The recurrence (37) is proved by invoking  $\beta$ -relation (29) to show the right-hand side here in the theorem is  $2a(\partial C_{n,0}(s, a)/\partial a)$  which equals the left-hand side. The recurrence (38) is easier, requiring simple integration by parts in the integral representation (20) for  $C$ .  $\square$

We are now prepared to establish a central result that will lead to a host of closed forms, which follows:

**Theorem 4.** *For any integer  $s$  and positive integer  $a$ , all the numbers*

$$(39) \quad C_{n,0}(s, a) := \int_{\vec{r} \in [0,1]^n} (a + r^2)^{s/2} \mathcal{D}\vec{r}$$

for  $n = 0, 1, 2$  are hyperclosed.

*Remark.* As with other parts of the present treatment, we not only prove hyperclosure, but do this constructively, so that an algorithm for achieving closed forms is implicit in the proof.

*Proof.*  $C_{0,0}(s, a) := a^{s/2}$  and  $C_{1,0}(s, a) = a^{s/2} {}_2F_1\left(\frac{1}{2}, -s/2; 3/2, -1/a\right)$  are clearly hyperclosed. So we turn our attention to  $C_{2,0}$ : For nonnegative even integer  $s$ , it is evident that the defining integral for  $C_{2,0}$  yields rational values. Consider, then, a single evaluation for negative even  $s$ , where we employ polar coordinates in the defining 2-dimensional integral to obtain

$$(40) \quad \begin{aligned} C_{2,0}(-2, a) &= \int_0^{\pi/4} dt (\log(a + \sec^2 t) - \log a) \\ &= -G + \text{Ti}_2\left(\frac{2+a-2\sqrt{1+a}}{a}\right) + \frac{\pi}{2} \log(1 + \sqrt{1+a}) - \frac{\pi}{4} \log a, \end{aligned}$$

where

$$(41) \quad G := \sum_{n \geq 0} \frac{(-1)^n}{(2n+1)^2} = \text{Ti}_2(1)$$

is the Catalan constant and as before  $Ti_2$  is the Lewin inverse-tangent integral; see (30), (31). Clearly  $C_{2,0}(-2, a)$  is hyperclosed for positive algebraic  $a$ . Now, in recurrence (37) with  $n = 2$ , there is a term  $C_{1,0}(s, a + 1)$  which we have seen to be hyperclosed. The recurrence thus reveals that  $C_{2,0}(-s, a)$  is hyperclosed for all negative even integers  $s$ .

It remains to handle all odd integers  $s$ . We observe another “ignition value”

$$(42) \quad C_{2,0}(1, a) = -\frac{1}{3}a^{3/2} \tan^{-1} \left( \frac{1}{\sqrt{a^2 + 2a}} \right) + \frac{1}{6}(3a + 1) \log \left( \frac{a + 2\sqrt{a+2} + 3}{a + 1} \right) + \frac{1}{3}\sqrt{a+2},$$

and this again drives the recurrence (37) to yield hyperclosure for any odd  $s$ .  $\square$

## 7. HYPERCLOSURE AND THE $B_n$

**Theorem 5** (Interrelations for the  $B_n$ ). *For integer  $n > 1$  and all complex  $s$ , we have a recurrence*

$$(43) \quad (n + s)(n + s - 1)B_n(s) = s(n + s - 2)B_n(s - 2) + n(n - 1)C_{n-2,0}(s, 2),$$

as well as various higher-order recurrences enjoying reduced indices on the  $C$ -functions; for example,

$$(44) \quad 2(s - 2)s(s + 1)B_5(s - 4) - (s + 3)\{s(3s + 7)B_5(s - 2) - (s + 4)(s + 5)B_5(s)\} = 60C_{2,0}(s, 3).$$

In addition, the residue  $\text{Res}_n$  of the unique pole at  $B_n(-n)$  is given for positive integers  $n$  by

$$(45) \quad \begin{aligned} \text{Res}_n &= nC_{n-1,0}(-n, 1) \\ &= -\frac{2}{n-2}B_n(-n+2) + \frac{n(n-1)}{n-2}C_{n-2,0}(2-n, 2); \quad n > 2. \end{aligned}$$

Finally, we have a special analytic-continuation value valid for all positive integers  $n$ :

$$(46) \quad B_n(-n-1) = -nC_{n-2,0}(1-n, 2).$$

*Remark.* In the instance  $s = -n$  where a pole is involved, an expression  $(n+s)B_n(s)$ , on the face of it  $0 \cdot \infty$ , is to be interpreted as the residue  $\text{Res}_n$  at the relevant pole. These residues allow us to effectively traverse  $B_n$ -poles when applying recurrence (43).

*Proof.* The first  $B_n, C$  recurrence (43) follows from the combination of proven relations (36) and (37). The second, higher-order recurrence is obtained by combining (37), (43). The residue formulae follow from (43) and (36).  $\square$

Theorem 5 allows us to evaluate important residues  $\text{Res}_n$ , at least for low-lying  $n$ . In fact, we remind ourselves that  $\text{Res}_n := \lim_{\epsilon \rightarrow 0} B_n(-n + \epsilon)$ , and state the residue

evaluations that were essential in rigorously establishing our tables of closed forms:

$$\begin{aligned}\text{Res}_1 &= 1, \text{Res}_2 = \frac{\pi}{2}, \\ \text{Res}_3 &= \frac{\pi}{2}, \text{Res}_4 = \frac{\pi^2}{8}, \\ \text{Res}_5 &= \frac{\pi^2}{12}.\end{aligned}$$

*Proof.* The evaluations for  $n = 1, 2$  are easy, using the first residue relation in Theorem 5. We then have

$$\begin{aligned}\text{Res}_3 &= -2B_3(-1) + 6C_{1,0}(-1, 2), \\ \text{Res}_4 &= -B_4(-2) + 6C_{2,0}(-2, 2), \\ \text{Res}_5 &= -\frac{4}{3}B_5(-3) - 4B_5(-1) + 10C_{2,0}(-1, 3).\end{aligned}$$

Each of these boils down to a rational times a power of  $\pi$  (we note that all four  $B$  values here are independently resolvable).  $\square$

Incidentally, we believe that  $\text{Res}_6 = \pi^3/64$ , and, remarkably, O-Y. Chan has recently conjectured a result that implies  $\text{Res}_7 = \pi^3/120$  with similar results for  $\text{Res}_{9,11,\dots}$ . In any case it seems reasonable to conjecture that in general,  $\text{Res}_n = Q_n \pi^{\lfloor n/2 \rfloor}$ , where  $Q_n$  is *rational*. Note that a proof of such a general conjecture would essentially yield an evaluation of any  $C_{m,0}(-m-1, 1)$ , for example, the specific conjecture about  $\text{Res}_7$  guesses a closed-form evaluation

$$\begin{aligned}C_{6,0}(-7, 1) &:= \int_0^1 \cdots \int_0^1 (1 + x_1^2 + \cdots x_6^2)^{-7/2} dx_1 \cdots dx_6 \\ &\stackrel{?}{=} \frac{\pi^3}{840}.\end{aligned}$$

We are now in a position to state a summary theorem about the box integrals  $B_n$ .

**Theorem 6** (Hyperclosure for specific  $B_n$ ). *For any integer  $s$ , each of*

$$B_1(s), B_2(s), B_3(s), B_4(s)$$

*is hyperclosed. As for 5 dimensions and integer  $s$ ,  $B_5(s)$  is hyperclosed except perhaps for  $s = -2, -4$ .*

*Remark.* Again, the proof following is constructive; i.e., gives rise to an immediate algorithm for generating closed forms. Note the exceptions  $s = -2, -4$  for  $n = 5$  dimensions; these exceptions represent the boundary of our current understanding of box integrals, even though these difficult cases may well be hyperclosed themselves.

*Proof.* From Theorem 4 it is immediate that  $B_m(s) = \frac{m}{m+s} C_{m-1,0}(s, 1)$  is hyperclosed for  $m = 1, 2, 3$ . So we turn to  $B_4$ , and observe that for nonnegative even integer  $s$ , the value  $B_4(s)$  is rational. From the first recurrence in Theorem 5, and knowledge of  $\text{Res}_4$ , we may take *one* value of  $B_4(\text{odd})$  and propagate that to *all*

other  $B_4(\text{odd})$ . The same goes for even arguments. Therefore, if we establish hyperclosure for  $B_4(-1)$  and  $B_4(-2)$ , say, then we know all  $B_4(\text{integer})$  to be hyperclosed via Theorem 4. To these ends, we observe

$$(47) \quad B_4(-1) = 2 \log 3 - \frac{2}{3} G + 2 \operatorname{Ti}_2(3 - 2\sqrt{2}) - \sqrt{8} \arctan\left(\frac{1}{\sqrt{8}}\right)$$

and

$$(48) \quad B_4(-2) = \pi \log(2 + \sqrt{3}) - 2G - \frac{\pi^2}{8}.$$

A proof of (48) starts with (25) and the evaluation of the jellium value  $J_4$  is given in our previous paper [5]; said proof thus reduces to showing that

$$\int_0^1 \frac{\log(3 + s^2)}{1 + s^2} ds = \frac{\pi}{4} \log(2 + \sqrt{3}) + \frac{\pi}{4} \log 2 - \operatorname{Ti}_2(-2 + \sqrt{3}) - G.$$

Using A2.2(3) in [19] this becomes

$$\int_0^1 \frac{\log(3 + s^2)}{1 + s^2} ds + \frac{\pi}{6} \log(2 + \sqrt{3}) - \frac{\pi}{4} \log 2 - \frac{1}{3} G = 0.$$

Now substituting  $s = \tan \theta$  yields an expression which computer algebra evaluates as

$$\frac{4}{3} G + \frac{\pi}{3} \log(2 + \sqrt{3}) - \operatorname{Ti}_2(2 + \sqrt{3}) - \operatorname{Ti}_2(2 - \sqrt{3}) = 0.$$

This is easily confirmed using [19, A2.2(3),(4)]. The proof of (47) is similarly completed; said proof reduces to resolving (70).

Finally, we handle the difficult case  $n = 5$ . One can prove that

$$\begin{aligned} B_5(1) &= \frac{1}{6} \sqrt{5} + \frac{1}{360} \pi^2 - \frac{4}{3} \sqrt{3} \arctan\left(\frac{1}{\sqrt{15}}\right) + \frac{10}{3} \log\left(\frac{\sqrt{5} + 1}{2}\right) \\ &\quad + \frac{7}{18} \left\{ \mathcal{K}_1 - \frac{\pi}{2} \log(2 + \sqrt{3}) \right\} \end{aligned}$$

and

$$\begin{aligned} B_5(-1) &= \frac{5}{3} \left\{ \mathcal{K}_1 - \frac{\pi}{2} \log(2 + \sqrt{3}) \right\} \\ &\quad + \frac{1}{48} \pi^2 - 5 \sqrt{6} \arctan\left(\frac{1}{\sqrt{15}}\right) + 5 \log\left(\frac{\sqrt{5} + 1}{2}\right) \end{aligned}$$

where  $\mathcal{K}_1$  is a certain definite integral that has been resolved; see our later section on  $\mathcal{K}$ -integrals. Now, employing recurrence (44), together with the known residue  $\operatorname{Res}_5$ , we can propagate this knowledge of  $B_5(\pm 1)$  to all  $B_5(\text{odd})$ .

As for even integer arguments, note from our tables that  $B_5(-6), B_5(-8)$  are independently resolved in terms of a hyperclosed integral  $\mathcal{K}_4$ . But, via the second recursion in Theorem 5, this means every  $B_5(-k)$  is hyperclosed for even integer  $k \geq 6$ . Thus the only exceptional instances out of all  $B_5(\text{integer})$  are  $B_5(-2), B_5(-4)$  as claimed.  $\square$

Another approach to recursions for  $B_n, \Delta_n$  as a function of  $s$  (for all positive integer  $n$ ) is via the linear differential equations satisfied by  $b$  and  $d$ ; see [12] and [11, p. 270]. This leads, for example, to an implementable 5-term recursion for  $B_4(s)$  in terms of  $B_4(s - 2), B_4(s - 4), B_4(s - 6), B_4(s - 8)$  with coefficients polynomial in  $s$ .

8. HYPERCLOSURE AND THE  $\Delta_n$ 

On the face of it, our definition (2) of the box integral  $\Delta_n$  would appear to present a  $(2n)$ -dimensional integration problem. But a certain  $n$ -fold integral suffices; in fact we have

$$(49) \quad \Delta_n(s) = 2^n \int_{\vec{r} \in [0,1]^n} r^s \prod_{k=1}^n (1 - r_k) \mathcal{D}\vec{r}.$$

This reduction from  $2n$  to  $n$  dimensions can be derived in various ways. Perhaps the most intuitive is to look at the probability density of a coordinate difference  $x = r_k - q_k$ , which turns out to be a triangle distribution with base  $[-1, 1]$  and height 1 at the origin-centered apex; i.e., the density is  $1 - |x|$ , and the new integral form follows.

It is interesting that (49) has the “leading term”  $2^n B_n(s)$  arising from the 1 component of the integrand’s product, indicating heuristically that  $\Delta_n$  and  $B_n$  should somehow be analytic relatives. Indeed, one can carry such an idea much further, to end up with powerful analytic expressions for  $\Delta_n(s)$ . Simple symmetries of the integrand in (49) reveal that

$$(50) \quad \Delta_n(s) = 2^n \sum_{k=0}^n \binom{n}{k} (-1)^k C_{n,k}(s, 0).$$

On the other hand, we have the recursion (38) that may be used to decrement both indices  $n, k$  on  $C_{n,k}$ . Thus we have the intriguing principle that  $\Delta_n$  can be formally expressed in terms of  $C_{m,0}$  functions, where  $m \leq n$ . But there is more: Some thought in regard to relations (36), (37), (43) reveals that the relevant  $C_{m,0}$  values lead back to the  $B_n$  box integrals, so that  $\Delta_n$  can be formally expressed in terms of the  $B_n$ . The summary result follows:

**Theorem 7** ( $\Delta_n$  as an analytic superposition of  $B_2, \dots, B_n$ ). *For arbitrary positive integer  $n$  and any complex  $s$ , we have an analytic superposition*

$$(51) \quad \Delta_n(s) = E_n(s) + \sum_{m=2}^n \sum_{j=1}^m R_{m,j}(s) B_m(s + 2n - 2j),$$

where  $E_n$  is an elementary function and each  $R_{m,j}$  is a rational-polynomial function.

*Remark.* Thus  $\Delta_n$  is in general a superposition of an  $E$  term and  $(n+2)(n-1)/2$  different  $B$  terms.

*Proof.* This result follows from the combinatorics embodied in relations (50), (36), (37), (43).  $\square$

Let us now give some entirely general analytic  $\Delta_n$  evaluations; first the easy case  $n = 1$ , for which the sum in Theorem 7 is empty and we have a simple, elementary function:

$$(52) \quad \Delta_1(s) = 2 \int_0^1 (1-x)x^2 dx = \frac{2}{1+s} - \frac{2}{2+s}.$$

Note the two poles, as we expect from previous analysis. Then from the combinatorics leading up to Theorem 7 we obtain

$$(53) \quad \Delta_2(s) = 8 \frac{(3+s)2^{\frac{s}{2}+1} + 1}{(s+2)(s+3)(s+4)} + 4B_2(s) - \frac{4(s+4)}{s+2} B_2(s+2).$$

Now note the existence of three poles (at  $s = -4, -3, -2$ ). Going yet deeper into the combinatorics, we have

$$(54) \quad \begin{aligned} \Delta_3(s) = & 24 \frac{(-3^{\frac{s}{2}+2}s + 2^{\frac{s}{2}+3})(s+5) + 1}{(s+2)(s+4)(s+5)(s+6)} + \frac{24}{s+2} B_2(s+2) \\ & - \frac{24(s+6)}{(s+2)(s+4)} B_2(s+4) + 8B_3(s) - \frac{12(s+5)}{s+2} B_3(s+2) \\ & + \frac{4(s+6)(s+7)}{(s+2)(s+4)} B_3(s+4). \end{aligned}$$

There are some difficulties attendant on this  $\Delta_3$  form; namely, the apparent pole at  $s = -2$  is specious. In order to get, such as, the  $\Delta_3(-2)$  closed form in our tables, one needs to take a careful limit  $s \rightarrow -2$ . Note also that the  $\Delta_3$  pole at  $s = -3$  is caused exclusively by the  $8B_3(s)$  term itself. Also, one needs a residue evaluation from Theorem 5 for the  $B_3(s+4)$  term at  $s = -7$ .

At the next level we obtain the complete analytic continuation for  $\Delta_4$ , in terms of  $B_2, B_3, B_4$ :

$$(55) \quad \begin{aligned} \Delta_4(s) = & 64 \frac{(3 \cdot 2^{\frac{s}{2}+3} + 2^{s+6} - 3^{\frac{s}{2}+4})(s+7) + 1}{(s+2)(s+4)(s+6)(s+7)(s+8)} \\ & + \frac{96}{(s+2)(s+4)} B_2(s+4) - \frac{96(s+8)}{(s+2)(s+4)(s+6)} B_2(s+6) \\ & + \frac{64}{s+2} B_3(s+2) - \frac{96(s+7)}{(s+2)(s+4)} B_3(s+4) \\ & + \frac{32(s+8)(s+9)}{(s+2)(s+4)(s+6)} B_3(s+6) + 16B_4(s) \\ & - \frac{88(s+6)}{3(s+2)} B_4(s+2) + \frac{8(s+8)(6s+43)}{3(s+2)(s+4)} B_4(s+4) \\ & - \frac{8(s+8)(s+9)(s+10)}{3(s+2)(s+4)(s+6)} B_4(s+6). \end{aligned}$$

Again the apparent pole at  $s = -2$  is specious, so one must work out another logarithmic limit in that case. For  $s = -9, -10$  we may use the known residues of the  $B$ -poles. (The poles at  $s = -4, -5, -6, -7, -8$  *do* exist; e.g. the term with  $B_3(s+2)$  has a pole at  $s = -5$ .)

Finally, as with lower dimensions, we can supply the following superposition formula for  $\Delta_5$  in terms of  $B_n$  with  $2 \leq n \leq 5$ ,

(56)

$$\begin{aligned} \Delta_5(s) = & 160 \frac{1 + (9+s)(2^{6+s/2} + 2^{10+s} - 5^{4+s/2} - 2 \cdot 3^{5+s/2})}{(2+s)(4+s)(6+s)(8+s)(9+s)(10+s)} \\ & + \frac{320}{(2+s)(4+s)(6+s)} B_2(6+s) - \frac{320(10+s)}{(2+s)(4+s)(6+s)(8+s)} B_2(8+s) \\ & + \frac{320}{(2+s)(4+s)} B_3(4+s) - \frac{480(9+s)}{(2+s)(4+s)(6+s)} B_3(6+s) \\ & + \frac{160(10+s)(11+s)}{(2+s)(4+s)(6+s)(8+s)} B_3(8+s) \\ & + \frac{160}{2+s} B_4(2+s) - \frac{880}{3} \frac{(8+s)}{(2+s)(4+s)} B_4(4+s) \\ & + \frac{80}{3} \frac{(10+s)(55+6s)}{(2+s)(4+s)(6+s)} B_4(6+s) \\ & - \frac{80}{3} \frac{(10+s)(11+s)(12+s)}{(2+s)(4+s)(6+s)(8+s)} B_4(8+s) \\ & + 32 B_5(s) - 200 \frac{(7+s)}{6+3s} B_5(2+s) + \frac{4}{3} \frac{(9+s)(291+35s)}{(2+s)(4+s)} B_5(4+s) \\ & - \frac{8}{3} \frac{(10+s)(11+s)(47+5s)}{(2+s)(4+s)(6+s)} B_5(6+s) \\ & + \frac{4}{3} \frac{(10+s)(11+s)(12+s)(13+s)}{(2+s)(4+s)(6+s)(8+s)} B_5(8+s). \end{aligned}$$

Such analytic formulae allow us to state a companion theorem to Theorem 6, as:

**Theorem 8** (Hyperclosure for specific  $\Delta_n$ ). *For any integer  $s$ , each of*

$$\Delta_1(s), \Delta_2(s), \Delta_3(s), \Delta_4(s)$$

*is hyperclosed. As for 5 dimensions and integer  $s$ ,  $\Delta_5(s)$  is hyperclosed except perhaps for  $s = -2, -4, -12$ .*

*Remark.* A summary of results here: With Theorem 6, we now know that  $B_{1,2,3,4}$  and  $\Delta_{1,2,3,4}$  are all hyperclosed at every integer argument, and that all  $B_5(\text{integer})$ ,  $D_5(\text{integer})$  are now proven hyperclosed, except for the short exception list

$$B_5(-2), B_5(-4), \Delta_5(-2), \Delta_5(-4), \Delta_5(-12).$$

It is especially interesting that the resolution of just *one* of  $B_5(-2)$ ,  $B_5(-4)$  would settle this whole exception list, because a certain linear combination of these two  $B_5$ 's is hyperclosed.

*Proof.* All of these hyperclosure results follow from the above analytic superpositions for  $\Delta_n$  in terms of  $B$ 's, together with knowledge of all relevant residues  $\text{Res}_n$ ,  $n = 1, 2, 3, 4, 5$ . In particular, for  $n = 5$ , the terms in (56) involving  $B_5$ 's have arguments  $s, s+2, s+4, s+6, s+8$ , so that whenever integer  $s \notin \{-2, -4, -12\}$ , only resolved  $B_5$ 's are involved. This established the set of three unresolved  $\Delta_5$ 's.  $\square$



9. DIFFICULTIES IN  $n \geq 5$  DIMENSIONS

We have not been able to obtain hyperclosure for all integer arguments for  $n = 5$  because of the finite exception list (see the Remark after Theorem 8). There may be some future hope in employing

$$(57) \quad \begin{aligned} (2+s)(4+s)B_5(s) &= 4 \int_0^{\pi/4} \int_0^{\pi/4} \int_0^1 (\sec^2(a) + \sec^2(b) + z^2)^{2+s/2} dz da db \\ &\quad - 2\pi \int_0^{\pi/4} {}_2F_1\left(\frac{1}{2}, -2 - \frac{s}{2}; \frac{3}{2}; -\cos^2(b)\right) \sec^{4+s}(b) db + \frac{1}{4} \frac{\pi^2}{5+s}. \end{aligned}$$

For integer  $s$  the integral in  $z$  can be performed symbolically and the hypergeometric function evaluated. This reduces  $B_5(s)$  to a double integral expression for  $s = -6$ , and also for  $s = -2, -4$  on applying the l'Hôpital rule.

As for the sutifying scenario of  $n = 6$  dimensions, we admit right off that we know not a *single* nontrivial closed form for a  $B_6$ . One might conceivably use

$$\begin{aligned} B_6(s) &= \frac{8}{(s+2)(s+4)(s+6)} \int_0^{\pi/4} \int_0^{\pi/4} \int_0^{\pi/4} (\sec^2 a + \sec^2 b + \sec^2 c)^{3+s/2} da db dc \\ &\quad - \frac{\pi}{2} \frac{3}{s+2} B_4(s+2) - \frac{\pi^2}{4} \frac{3}{(s+2)(s+4)} B_2(s+4), \end{aligned}$$

valid for all values of  $s$ . In particular,

$$\begin{aligned} B_6(-7) &= - \frac{8}{15} \int_0^{\pi/4} \int_0^{\pi/4} \int_0^{\pi/4} \frac{da db dc}{\sqrt{\sec^2(a) + \sec^2(b) + \sec^2(c)}} \\ &\quad + \frac{3\sqrt{2}}{5} \arctan\left(\frac{1}{\sqrt{8}}\right) \pi + \frac{3\sqrt{2}}{32} \pi^2. \end{aligned}$$

Moreover, the triple integral above resolves to

$$\begin{aligned} &\frac{1}{2} \int_0^{\pi/4} \int_0^{\pi/4} \frac{\operatorname{arcsec}(1 + \sec^2(a) + \sec^2(b))}{\sqrt{\sec^2(a) + \sec^2(b)}} da db \\ &= -\frac{3}{4} \int_1^2 \frac{\operatorname{arcsec}(z+3) \operatorname{arcsec}(z)}{(z+2)^{3/2} \sqrt{z+1}} dz \\ &\quad + \frac{\pi}{\sqrt{8}} \left\{ 2 \arctan\left(\frac{3}{4}\right) - 3 \arctan\left(\frac{7}{8} \sqrt{2}\right) + \sqrt{\frac{3}{2}} \arctan(2\sqrt{6}) \right\}. \end{aligned}$$

Thus we arrive at

$$(58) \quad \begin{aligned} B_6(-7) &= \frac{2}{5} \mathcal{K}_8 + \frac{7\sqrt{2}}{60} \pi^2 - \frac{7\sqrt{2}}{5} \pi \arctan\left(\frac{1}{\sqrt{8}}\right) + \frac{8\sqrt{2}}{15} \pi \arctan\left(\frac{1}{2}\right) \\ &\quad - \frac{2\sqrt{3}}{15} \pi \arctan(\sqrt{24}) \end{aligned}$$

where an integral form of  $\mathcal{K}_8$ —an integral still unresolved, to our knowledge—is exhibited in the next section.

10.  $\mathcal{K}$ -INTEGRALS

In a set of marvelous preprints, G. Lamb [17] managed to resolve some “dangling integrals” from our previous work [5]. We called these  $\mathcal{K}_m$ , for  $m = 0, 1, 2, 3$ . Now,

via the combination of proof via alternative integration (as with result (69) below), together with the powerful Lamb techniques, we know closed forms such as

$$(59) \quad \mathcal{K}_0 := \int_0^1 \frac{\operatorname{arctanh}\left(\frac{1}{\sqrt{3+y^2}}\right)}{1+y^2} dy = \frac{3}{2} \operatorname{Ti}_2(3-2\sqrt{2}) + \frac{\pi}{4} \log(1+\sqrt{2}) - \frac{1}{2}G.$$

Thus  $\mathcal{K}_0$  is hyperclosed.

The next integral is perhaps the most difficult one of the present treatment. Along the way to the following answer—having started with the Lamb method—were stages of symbolics, at times for us involving expressions of over  $10^4$  characters in modern symbolic processing:

$$(60) \quad \begin{aligned} \mathcal{K}_1 &:= \int_3^4 \frac{\operatorname{arcsec}(x)}{\sqrt{x^2-4x+3}} dx \\ &= \operatorname{Cl}_2(\theta) - \operatorname{Cl}_2\left(\theta + \frac{\pi}{3}\right) - \operatorname{Cl}_2\left(\theta - \frac{\pi}{2}\right) + \operatorname{Cl}_2\left(\theta - \frac{\pi}{6}\right) - \operatorname{Cl}_2\left(3\theta + \frac{\pi}{3}\right) \\ &\quad + \operatorname{Cl}_2\left(3\theta + \frac{2\pi}{3}\right) - \operatorname{Cl}_2\left(3\theta - \frac{5\pi}{6}\right) + \operatorname{Cl}_2\left(3\theta + \frac{5\pi}{6}\right) \\ &\quad + \left(6\theta - \frac{5\pi}{2}\right) \log(2-\sqrt{3}). \end{aligned}$$

where

$$3\theta := \arctan\left(\frac{16-3\sqrt{15}}{11}\right) + \pi.$$

It may well be that this closed form for  $\mathcal{K}_1$  can be further simplified.

Not so hard, but certainly nontrivial, is

$$(61) \quad \begin{aligned} \mathcal{K}_2 &:= \int_0^{\pi/4} \sqrt{1+\sec^2(a)} \arctan\left(\frac{1}{\sqrt{1+\sec^2(a)}}\right) da \\ &= \frac{1}{2} \operatorname{Ti}_2(-2+\sqrt{3}) + \frac{\pi}{8} \log(2+\sqrt{3}) + \frac{\pi^2}{32}. \end{aligned}$$

Finally, we have resolved a dangling integral from [5] involving dimension  $n=5$ , as

$$(62) \quad \begin{aligned} \mathcal{K}_3 &:= \int_0^{\pi/4} \int_0^{\pi/4} \sqrt{1+\sec^2(a)+\sec^2(b)} da db \\ &= \frac{1}{4} \log(2+\sqrt{3}) + \frac{1}{48} \pi^2 - \frac{1}{10} B_5(-3). \end{aligned}$$

Indeed, the formula for the jellium constant  $J_5$  given in [5, §7.3] yields precisely (62) and the closed form for  $B_5(-3)$  is listed in Table 4.

Moving on, we hereby define additional  $\mathcal{K}$ -integrals, starting with

$$(63) \quad \mathcal{K}_4 := \int_0^{\pi/4} \frac{\arctan\left(\frac{1}{\sqrt{2+\sec^2(t)}}\right)}{\sqrt{2+\sec^2(t)}} dt$$

and

$$(64) \quad \mathcal{K}_5 := \int_0^{\pi/4} \int_0^{\pi/4} \log(1 + \sec^2(a) + \sec^2(b)) \, da \, db.$$

Following suggestions in [18] and significant symbolic computation, we express  $\mathcal{K}_4$  explicitly in terms of complex dilogarithms. The computer algebra system produced an answer, which with considerable massaging became

$$(65) \quad \begin{aligned} \frac{1}{\sqrt{8}} \mathcal{K}_4 = & \frac{7\pi}{16} \arctan(2) + \frac{3\pi}{16} \arctan(27 + 20\sqrt{2}) - \frac{13\pi^2}{64} \\ & + \frac{1}{8} \Re \left\{ \operatorname{Li}_2(\sqrt{2} + i) - \operatorname{Li}_2(-\sqrt{2} + i) \right\} \\ & + \frac{1}{4} \Re \left\{ \operatorname{Li}_2\left(\frac{4}{5} - \frac{3}{5}i - \frac{3}{5}\sqrt{2} - \frac{4}{5}i\sqrt{2}\right) \right. \\ & \quad \left. - \operatorname{Li}_2\left(\frac{4}{5} - \frac{3}{5}i + \frac{3}{5}\sqrt{2} + \frac{4}{5}i\sqrt{2}\right) \right\} \\ & + \frac{1}{8} \Re \left\{ \operatorname{Li}_2\left(\frac{4}{15} - \frac{1}{5}i - \frac{1}{5}\sqrt{2} - \frac{4}{15}i\sqrt{2}\right) \right. \\ & \quad \left. - \operatorname{Li}_2\left(\frac{4}{15} - \frac{1}{5}i + \frac{1}{5}\sqrt{2} + \frac{4}{15}i\sqrt{2}\right) \right\}. \end{aligned}$$

The arguments of the dilogarithms here solve an interesting, degree-12 polynomial system. One may use dilogarithm reflection formulae to obtain closed forms such as

$$(66) \quad \begin{aligned} \sqrt{8} \mathcal{K}_4 = & -\operatorname{Li}_2\left(\frac{1}{\sqrt{3}}, \theta\right) + \operatorname{Li}_2\left(\frac{1}{\sqrt{3}}, \pi - \theta\right) - \operatorname{Li}_2\left(\frac{1}{\sqrt{3}}, \pi - \alpha\right) + \operatorname{Li}_2\left(\frac{1}{\sqrt{3}}, \beta\right) \\ & + (\pi - 8\theta) \arctan\left(\frac{1}{2}\right), \end{aligned}$$

where

$$\theta := \arctan\left(\frac{1}{\sqrt{2}}\right), \quad \alpha := \arctan\left(\frac{3 + 4\sqrt{2}}{-4 + 3\sqrt{2}}\right) \text{ and } \beta := \arctan\left(\frac{-3 + 4\sqrt{2}}{4 + 3\sqrt{2}}\right),$$

with the Lewin generalization  $\operatorname{Li}_2(r, \phi) := \Re \operatorname{Li}_2(re^{i\phi})$ ; see [19, A2.5 (1)]. It is immediate that  $\mathcal{K}_4$  is hyperclosed, since in our  $\mathcal{K}_4$  formulae any arguments  $re^{\pm i\theta}$  are all algebraic, and  $2\Re \operatorname{Li}_2(z) = \operatorname{Li}_2(z) + \operatorname{Li}_2(z^*)$ .

So, we know that  $\mathcal{K}_{0,1,2,3,4}$  are all hyperclosed, but we do not know this for  $\mathcal{K}_5$ . Various recondite, but alas partial results can be derived, starting typically from (64) and employing coordinates  $\tan a, \tan b$  over the unit 2-square. One can obtain such a 1-dimensional-integral dependence

$$(67) \quad \begin{aligned} \mathcal{K}_5 = & \int_0^1 \frac{\arctan(\sqrt{t}) \arctan\left(\frac{1}{\sqrt{3+t}}\right)}{\sqrt{3+t}(2+t)} dt - \frac{\pi}{2} G + \frac{\pi^2}{16} \log 3 \\ & + \frac{\pi}{2} (3 - \sqrt{8}) \operatorname{Ti}_2(3 - \sqrt{8}) + \frac{\pi}{12} \operatorname{Ti}_2\left(\frac{1}{3}\right) + \frac{\pi^2}{8} \log(\sqrt{2} - 1), \end{aligned}$$

or an efficient sum

$$\mathcal{K}_5 = \frac{\pi^2}{16} \log 3 - \sum_{m \geq 1} \frac{1}{m 3^m} \sum_{j=0}^m \binom{m}{j} \left(h_j - \frac{\pi}{4}\right) \left(h_{m-j} - \frac{\pi}{4}\right),$$

where  $h_k := 1 - 1/3 + 1/5 - \cdots \pm 1/(2j-1)$ , with  $h_0 := 0$ . This summatory representation allows extreme-precision evaluation of  $\mathcal{K}_5$  without recourse to quadrature per se.

Now to the concept of alternative integration: It is highly interesting that the box-integral theory can sometimes be used to resolve previously unknown integrals that have, on the face of it, little to do with  $n$ -dimensional boxes. A canonical example is the case of  $\Delta_3(-2)$ , which is obtained through the rather delicate limit process  $s \rightarrow -2$  in (54) in order to complete hyperclosure for  $n = 3$ . But when we attempted to evaluate  $\Delta_3(-2)$  from the alternative formula

$$(68) \quad \Delta_3(-2) = 8 \int_{\vec{r} \in [0,1]^3} \frac{(1-x)(1-y)(1-z)}{x^2 + y^2 + z^2} dx dy dz,$$

we ended up with a single, troublesome arctan integral as the “dangling term”. But the ( $s \rightarrow -2$ ) limit procedure does a complete hypergeometric breakdown, and all of this proves the result

$$(69) \quad \begin{aligned} \mathcal{K}_6 &:= \int_0^1 \sqrt{1+z^2} \arctan\left(\frac{1}{\sqrt{1+z^2}}\right) dz \\ &= \frac{1}{2} - \frac{G}{2} + \frac{\pi}{4} \log(1+\sqrt{2}) + \frac{1}{2} \text{Ti}_2(3-2\sqrt{2}). \end{aligned}$$

We do not give here a direct proof of this integral relation, although G. Lamb has now provided a fine analytic evaluation of  $\mathcal{K}_6$ ; see [18]. Another example of an indirect integral resolution is

$$(70) \quad \begin{aligned} \mathcal{K}_7 &:= \int_0^{\pi/4} \log(1 + \sqrt{2 + \sec^2 t}) dt \\ &= -G + 2 \text{Ti}_2(3-2\sqrt{2}) + \frac{\pi}{2} \log(1+\sqrt{2}). \end{aligned}$$

Finally, we define

$$(71) \quad \mathcal{K}_8 := \int_1^2 \frac{\text{arcsec}(x+3) \text{arcsec}(x)}{\sqrt{(x+1)(x+2)^3}} dx,$$

and observe that  $\mathcal{K}_8$ , along with the elusive  $\mathcal{K}_5$ , are the only unresolved instances of our integrals  $\mathcal{K}_{0,1,\dots,8}$ .

Again, knowledge of  $\mathcal{K}_8$  would give us  $B_6(-7)$ , as in (58), while hyperclosure of  $\mathcal{K}_5$  would establish hyperclosure of *all*  $B_5(\text{integer})$ ,  $\Delta_5(\text{integer})$ .

## 11. CURIOSITIES

One new result of some interest is that another unphysical, but valid analytically continued value discussed in our previous work [5], namely

$$B_4(-5) = -0.961203932689953457121659780024745 \dots$$

is now known in closed form. In fact, this previously mysterious analytic-continuation value is  $-\sqrt{8} \arctan(1/\sqrt{8})$  (see Tables and the last part of Theorem 5). However, there are still many unexplained empirical phenomena. For example, we do *not* know in closed form the zero of  $\Delta_2(s)$  at

$$s = -5.1378771851212623537 \dots,$$

though we have developed herein enough machinery to find this zero to extreme precision. (See Figure 1 for a pictorial of the zero.) Moreover, we are not aware of any other zeros in  $n = 2$  or any other dimension; evidently, this zero of  $\Delta_2$  is some kind of anomaly. There is also an empirical local minimum for  $B_2$ , at

$$s = 3.6675667756027541433 \dots,$$

and again a closed form is unknown.

Another curiosity is that some statistical quantities over the hypercube are almost trivial to resolve. For example, the exponential expectations

$$E_n(\lambda) := \langle e^{-\lambda^2 |\vec{r}|^2} \rangle_{\vec{r} \in [0,1]^n},$$

$$F_n(\lambda) := \langle e^{-\lambda^2 |\vec{r} - \vec{q}|^2} \rangle_{\vec{r}, \vec{q} \in [0,1]^n},$$

for constant  $\lambda$  do *not* need to be obtained from a generating function or series or anything complicated. Instead, closed forms are immediate, based on the defining relations (3), (4):

$$E_n(\lambda) = b^n(\lambda) = \left( \frac{\pi}{2\lambda} \right)^n \operatorname{erf}^n(\lambda),$$

$$F_n(\lambda) = d^n(\lambda).$$

The allure of such closed forms is that they hold in all dimensions, and may well replace the box integrals  $B_n(s), \Delta_n(s)$  as the right tools to assess the statistical character of point clouds, again as in reference [14]. In spite of this streamlined approach to cloud measures, it seems (heuristically) that both of

$$\langle e^{-\kappa |\vec{r}|} \rangle_{\vec{r} \in [0,1]^n}, \quad \langle e^{-\kappa |\vec{r} - \vec{q}|} \rangle_{\vec{r}, \vec{q} \in [0,1]^n}$$

should be extremely difficult to evaluate in any general way. Even if one were to revert to series expansion of the exponential, one would need  $B_n(s)$  for all non-negative integers  $s$ , yet we have met with extreme difficulties when  $n > 5$ . This is not to claim some clever prescription—a novel use of recurrences, or differential relations—would not solve this problem.

And what about noninteger arguments for the box integrals? One might extend the definition of hypergeometric closure based on such findings as

$$(72) \quad B_3\left(-\frac{7}{2}\right) = -2\pi - \frac{8}{5 \cdot 2^{\frac{1}{4}}} F_1\left(\frac{5}{4}; \frac{1}{2}, \frac{3}{4}; \frac{9}{4}; \frac{1}{2}, -\frac{1}{2}\right) \\ + \frac{16}{5} \sqrt{\pi} \frac{\Gamma(\frac{9}{4})}{\Gamma(\frac{7}{4})} {}_2F_1\left(\frac{5}{4}, \frac{3}{4}; \frac{7}{4}; -1\right).$$

Here,  $F_1$  is the Appell hypergeometric function defined as a series in two variables [2]. Thus we expect entities such as  $B_3(\text{odd}/2)$  to involve the Appell hypergeometric. Such examples suggest that there might be a kind of higher level of hypergeometric-closure theory for noninteger rational arguments  $s$ .

TABLE 1. Some relatively easy evaluations for  $B_n(s)$ . Every  $B_k(\text{integer})$  for  $k=1, 2$  can be given a closed form (see Theorem 6).

$n$	$s$	$B_n(s)$
any	even $\geq 0$	rational: $B_2(2) = 2/3$
1	-1	$\infty$
1	any	$\frac{1}{s+1}$
2	-4	$-\frac{1}{4} - \frac{\pi}{8}$
2	-3	$-\sqrt{2}$
2	-2	$\infty$
2	-1	$2 \log(1 + \sqrt{2})$
2	1	$\frac{1}{3}\sqrt{2} + \frac{1}{3} \log(1 + \sqrt{2})$
2	3	$\frac{7}{20}\sqrt{2} + \frac{3}{20} \log(1 + \sqrt{2})$
2	any	$\frac{2}{2+s} {}_2F_1\left(\frac{1}{2}, -\frac{s}{2}; \frac{3}{2}; -1\right)$

TABLE 2. Example evaluations of  $B_3(s)$ . Every  $B_3(\text{integer})$  can be given a closed form, being as we can express every  $B_3$  in terms of a function  $C_{2,0}$  which we have shown to be hyperclosed at relevant arguments.

$n$	$s$	$B_n(s)$
3	-5	$-\frac{1}{6}\sqrt{3} - \frac{1}{12}\pi$
3	-4	$-\frac{3}{2}\sqrt{2} \arctan \frac{1}{\sqrt{2}}$
3	-3	$\infty$
3	-2	$-3G + \frac{3}{2}\pi \log(1 + \sqrt{2}) + 3 \operatorname{Ti}_2(3 - 2\sqrt{2})$
3	-1	$-\frac{1}{4}\pi + \frac{3}{2} \log(2 + \sqrt{3})$
3	1	$\frac{1}{4}\sqrt{3} - \frac{1}{24}\pi + \frac{1}{2} \log(2 + \sqrt{3})$
3	3	$\frac{2}{5}\sqrt{3} - \frac{1}{60}\pi + \frac{7}{20} \log(2 + \sqrt{3})$
3	any	Integral representation (23), relation (36)

TABLE 3. Example evaluations of  $B_4(s)$ . Every  $B_4(\text{integer})$  can be given a closed form, on the basis of recursions and “ignition values” such as the pair  $B_4(-1), B_4(-2)$ .

$n$	$s$	$B_n(s)$
4	-5	$-\sqrt{8} \arctan\left(\frac{1}{\sqrt{8}}\right)$
4	-4	$\infty$
4	-3	$4G - 12\text{Ti}_2(3 - 2\sqrt{2})$
4	-2	$\pi \log(2 + \sqrt{3}) - 2G - \frac{\pi^2}{8}$
4	-1	$2\log 3 - \frac{2}{3}G + 2\text{Ti}_2(3 - 2\sqrt{2}) - \sqrt{8} \arctan\left(\frac{1}{\sqrt{8}}\right)$
4	1	$\frac{2}{5} - \frac{G}{10} + \frac{3}{10}\text{Ti}_2(3 - 2\sqrt{2}) + \log 3 - \frac{7\sqrt{2}}{10} \arctan\left(\frac{1}{\sqrt{8}}\right)$
4	any	Integral representation (25), recursions (43)

TABLE 4. Example evaluations of  $B_5(s)$ . Here  $\theta = \arctan((16 - 3\sqrt{15})/11)$ . We have proven that every  $B_5(\text{odd})$  is hyperclosed. Note that  $\mathcal{K}_4$  here is known, hyperclosed; yet, an unresolved (“dangling”) integral  $K_5$  is *not* yet known to be hyperclosed, but may well be. A hyperclosure proof for  $\mathcal{K}_5$  would serve to establish all the  $B_5(\text{even})$  by settling  $B_5(-2), B_5(-4)$ , leading thus to resolution of all  $B_n(\text{integer}), \Delta_n(\text{integer})$  for  $n = 1, 2, 3, 4, 5$ .

$n$	$s$	$B_n(s)$
5	-8	$\frac{25}{36}\mathcal{K}_4 - \frac{25}{288}\pi\sqrt{2}\arctan\left(\frac{1}{\sqrt{2}}\right) - \frac{5}{72}\arctan\left(\frac{1}{2}\right)$
5	-7	$-\frac{1}{\sqrt{3}}\arctan\left(\frac{1}{\sqrt{15}}\right) - \frac{1}{120}\pi^2$
5	-6	$5\mathcal{K}_4 - \frac{5}{8}\pi\sqrt{2}\arctan\left(\frac{1}{\sqrt{2}}\right)$
5	-5	$\infty$
5	-4	$-5\mathcal{K}_5 - \frac{5}{2}\pi G + \frac{5}{4}\pi^2 \log(1 + \sqrt{2}) + \frac{5}{2}\pi\text{Ti}_2(3 - 2\sqrt{2})$
5	-3	$\frac{110}{9}G - 10\log(2 - \sqrt{3})\theta - \frac{1}{8}\pi^2 - 10\text{Cl}_2\left(\frac{1}{3}\theta + \frac{1}{3}\pi\right) + 10\text{Cl}_2\left(\frac{1}{3}\theta - \frac{1}{6}\pi\right) + \frac{10}{3}\text{Cl}_2\left(\theta + \frac{1}{6}\pi\right) + \frac{20}{3}\text{Cl}_2\left(\theta + \frac{4}{3}\pi\right) - \frac{10}{3}\text{Cl}_2\left(\theta + \frac{5}{3}\pi\right) - \frac{20}{3}\text{Cl}_2\left(\theta + \frac{11}{6}\pi\right)$
5	-2	$\frac{8}{3}B_5(-6) - \frac{1}{3}B_5(-4) + \frac{5}{2}\pi\log 3 + 10\text{Ti}_2\left(\frac{1}{3}\right) - 10G$
5	-1	$-\frac{110}{27}G + \frac{10}{3}\theta\log(2 - \sqrt{3}) + \frac{1}{48}\pi^2 + 5\log\left(\frac{1+\sqrt{5}}{2}\right) - \frac{5}{2}\sqrt{3}\arctan\left(\frac{1}{\sqrt{15}}\right) + \frac{10}{3}\text{Cl}_2\left(\frac{1}{3}\theta + \frac{1}{3}\pi\right) - \frac{10}{3}\text{Cl}_2\left(\frac{1}{3}\theta - \frac{1}{6}\pi\right) - \frac{10}{9}\text{Cl}_2\left(\theta + \frac{1}{6}\pi\right) - \frac{20}{9}\text{Cl}_2\left(\theta + \frac{4}{3}\pi\right) + \frac{10}{9}\text{Cl}_2\left(\theta + \frac{5}{3}\pi\right) + \frac{20}{9}\text{Cl}_2\left(\theta + \frac{11}{6}\pi\right)$
5	1	$-\frac{77}{81}G + \frac{7}{9}\theta\log(2 - \sqrt{3}) + \frac{1}{360}\pi^2 + \frac{1}{6}\sqrt{5} + \frac{10}{3}\log\left(\frac{1+\sqrt{5}}{2}\right) - \frac{4}{3}\sqrt{3}\arctan\left(\frac{1}{\sqrt{15}}\right) + \frac{10}{9}\text{Cl}_2\left(\frac{1}{3}\theta + \frac{1}{3}\pi\right) - \frac{7}{9}\text{Cl}_2\left(\frac{1}{3}\theta - \frac{1}{6}\pi\right) - \frac{7}{27}\text{Cl}_2\left(\theta + \frac{1}{6}\pi\right) - \frac{14}{27}\text{Cl}_2\left(\theta + \frac{4}{3}\pi\right) + \frac{7}{27}\text{Cl}_2\left(\theta + \frac{5}{3}\pi\right) + \frac{14}{27}\text{Cl}_2\left(\theta + \frac{11}{6}\pi\right)$
5	any odd	Closed forms follow from recursion (43), using residues as needed
5	any even	Closed forms follow from recursion (43), using residues as needed, with only $B_5(-2), B_5(-4)$ remaining unresolved.

TABLE 5. Some relatively easy evaluations for  $\Delta_n(s)$ . Every  $\Delta_k(\text{integer})$  for  $k = 1, 2$  can be given a closed form (see Theorem 8). (Note: The closed form for  $\Delta_2(-1)$  here has been repaired w.r.t. the previous work [5].)

$n$	$s$	$\Delta_n(s)$
any	even $\geq 0$	rational: $\Delta_2(2) = 1/3$
1	-1, -2	$\infty$
1	any	$\frac{2}{s+1} - \frac{2}{s+2}$
2	-5	$\frac{4}{3} + \frac{8}{9}\sqrt{2}$
2	-2, -3, -4	$\infty$
2	-1	$\frac{4}{3} - \frac{4}{3}\sqrt{2} + 4\log(1 + \sqrt{2})$
2	1	$\frac{2}{15} + \frac{1}{15}\sqrt{2} + \frac{1}{3}\log(1 + \sqrt{2})$
2	any	Formula (53), using known $B_n$ -residues as needed

TABLE 6. Example evaluations for  $\Delta_3(s)$ . Every  $\Delta_3(\text{integer})$  can be given a closed form (see Theorem 8).

$n$	$s$	$\Delta_n(s)$
3	-7	$\frac{4}{5} - \frac{16\sqrt{2}}{15} + \frac{2\sqrt{3}}{5} + \frac{\pi}{15}$
3	3, -4, -5, -6	$\infty$
3	-2	$2\pi - 12G + 12\text{Ti}_2(3 - 2\sqrt{2}) + 6\pi\log(1 + \sqrt{2}) + 2\log 2 - \frac{5}{2}\log 3 - 8\sqrt{2}\arctan\left(\frac{1}{\sqrt{2}}\right)$
3	-1	$\frac{2}{5} - \frac{2}{3}\pi + \frac{2}{5}\sqrt{2} - \frac{4}{5}\sqrt{3} + 2\log(1 + \sqrt{2}) + 12\log\left(\frac{1+\sqrt{3}}{\sqrt{2}}\right) - 4\log(2 + \sqrt{3})$
3	1	$-\frac{118}{21} - \frac{2}{3}\pi + \frac{34}{21}\sqrt{2} - \frac{4}{7}\sqrt{3} + 2\log(1 + \sqrt{2}) + 8\log\left(\frac{1+\sqrt{3}}{\sqrt{2}}\right)$
3	3	$-\frac{1}{105} - \frac{2}{105}\pi + \frac{73}{840}\sqrt{2} + \frac{1}{35}\sqrt{3} + \frac{3}{56}\log(1 + \sqrt{2}) + \frac{13}{35}\log\left(\frac{1+\sqrt{3}}{\sqrt{2}}\right)$
3	any	Formula (54), using known $B_n$ -residues as needed



TABLE 7. Example evaluations for  $\Delta_4(s)$ . Every  $\Delta_4(\text{integer})$  can be given a closed form (see Theorem 8).

$n$	$s$	$\Delta_n(s)$
4	$-4, \dots, -8$	$\infty$
4	-3	$-\frac{128}{15} + \frac{16}{3} \pi - 8 \log(1 + \sqrt{2}) - 32 \log(1 + \sqrt{3}) + 16 \log 2 + 20 \log 3$ $-\frac{8}{5} \sqrt{2} + \frac{32}{5} \sqrt{3} - 32 \sqrt{2} \arctan\left(\frac{1}{\sqrt{8}}\right) - 96 \text{Ti}_2(3 - 2\sqrt{2}) + 32 G$
4	-2	$-\frac{16}{15} \pi \sqrt{3} - \frac{8}{3} \pi \log 2 + \frac{16}{3} \pi \log(1 + \sqrt{3}) - \frac{2}{3} \pi^2 + \frac{4}{5} \pi + \frac{8}{5} \sqrt{2} \arctan(2\sqrt{2})$ $+\frac{2}{5} \log 3 - 4 \pi \log(\sqrt{2} - 1) + 8 \text{Ti}_2(3 - 2\sqrt{2}) - \frac{40}{3} G - \frac{8}{3} \log 2$
4	-1	$-\frac{152}{315} - \frac{8}{15} \pi - \frac{16}{5} \log 2 + \frac{2}{5} \log 3 + \frac{68}{105} \sqrt{2} - \frac{16}{35} \sqrt{3} + \frac{4}{5} \log(1 + \sqrt{2})$ $+\frac{32}{5} \log(1 + \sqrt{3}) - \frac{8}{3} G + 8 \text{Ti}_2(3 - 2\sqrt{2}) - \frac{8}{5} \sqrt{2} \arctan(\sqrt{2}/4)$
4	1	$-\frac{23}{135} - \frac{16}{315} \pi - \frac{52}{105} \log 2 + \frac{197}{420} \log 3 + \frac{73}{630} \sqrt{2} + \frac{8}{105} \sqrt{3}$ $+\frac{1}{14} \log(1 + \sqrt{2}) + \frac{104}{105} \log(1 + \sqrt{3}) - \frac{68}{105} \sqrt{2} \arctan\left(\frac{1}{\sqrt{8}}\right) - \frac{4}{15} G$ $+\frac{4}{5} \text{Ti}_2(3 - 2\sqrt{2})$
4	any	Formula (55), using known $B_n$ -residues as needed

 TABLE 8. Example evaluations of  $\Delta_5(s)$ . It is proven that every  $\Delta_5(\text{odd})$  is hyperclosed. Every  $\Delta_5(\text{even})$  is hyperclosed, with perhaps three exceptions as in the table.

$n$	$s$	$\Delta_n(s)$
5	$-5, \dots, -10$	$\infty$
5	1	$-\frac{1279}{567} G - \frac{4}{189} \pi + \frac{4}{315} \pi^2 - \frac{449}{3465} + \frac{3239}{62370} \sqrt{2} + \frac{568}{3465} \sqrt{3} - \frac{380}{6237} \sqrt{5}$ $+\frac{295}{252} \log 3 + \frac{1}{54} \log(1 + \sqrt{2}) + \frac{20}{63} \log(2 + \sqrt{3}) + \frac{64}{189} \log\left(\frac{1 + \sqrt{5}}{2}\right)$ $-\frac{73}{63} \sqrt{2} \arctan\left(\frac{1}{\sqrt{8}}\right) - \frac{8}{21} \sqrt{3} \arctan\left(\frac{1}{\sqrt{15}}\right) + \frac{104}{63} \log(2 - \sqrt{3}) \theta$ $+\frac{2}{7} \text{Ti}_2(3 - 2\sqrt{2}) + \frac{104}{63} \text{Cl}_2\left(\frac{1}{3} \theta + \frac{1}{3} \pi\right) - \frac{104}{63} \text{Cl}_2\left(\frac{1}{3} \theta - \frac{1}{6} \pi\right)$ $-\frac{104}{189} \text{Cl}_2\left(\theta + \frac{1}{6} \pi\right) - \frac{208}{189} \text{Cl}_2\left(\theta + \frac{4}{3} \pi\right) + \frac{104}{189} \text{Cl}_2\left(\theta + \frac{5}{3} \pi\right) + \frac{208}{189} \text{Cl}_2\left(\theta + \frac{11}{6} \pi\right)$
5	any odd	Closed forms follow from (56), using residues as needed
5	any even	Closed forms follow from (56), using residues as needed, with only $\Delta_5(-2), \Delta_5(-4), \Delta_5(-12)$ remaining unresolved.

TABLE 7. Example evaluations for  $\Delta_4(s)$ . Every  $\Delta_4(\text{integer})$  can be given a closed form (see Theorem 8).

$n$	$s$	$\Delta_n(s)$
4	$-4, \dots, -8$	$\infty$
4	-3	$-\frac{128}{15} + \frac{16}{3}\pi - 8 \log(1 + \sqrt{2}) - 32 \log(1 + \sqrt{3}) + 16 \log 2 + 20 \log 3$ $-\frac{8}{5}\sqrt{2} + \frac{32}{5}\sqrt{3} - 32\sqrt{2} \arctan\left(\frac{1}{\sqrt{8}}\right) - 96 \text{Ti}_2(3 - 2\sqrt{2}) + 32G$
4	-2	$-\frac{16}{15}\pi\sqrt{3} - \frac{8}{3}\pi \log 2 + \frac{16}{3}\pi \log(1 + \sqrt{3}) - \frac{2}{3}\pi^2 + \frac{4}{5}\pi + \frac{8}{5}\sqrt{2} \arctan(2\sqrt{2})$ $+\frac{2}{5}\log 3 - 4\pi \log(\sqrt{2} - 1) + 8\text{Ti}_2(3 - 2\sqrt{2}) - \frac{40}{3}G - \frac{8}{3}\log 2$
4	-1	$-\frac{152}{315} - \frac{8}{15}\pi - \frac{16}{5}\log 2 + \frac{2}{5}\log 3 + \frac{68}{105}\sqrt{2} - \frac{16}{35}\sqrt{3} + \frac{4}{5}\log(1 + \sqrt{2})$ $+\frac{32}{5}\log(1 + \sqrt{3}) - \frac{8}{3}G + 8\text{Ti}_2(3 - 2\sqrt{2}) - \frac{8}{5}\sqrt{2} \arctan(\sqrt{2}/4)$
4	1	$-\frac{23}{135} - \frac{16}{315}\pi - \frac{52}{105}\log 2 + \frac{197}{420}\log 3 + \frac{73}{630}\sqrt{2} + \frac{8}{105}\sqrt{3}$ $+\frac{1}{14}\log(1 + \sqrt{2}) + \frac{104}{105}\log(1 + \sqrt{3}) - \frac{68}{105}\sqrt{2} \arctan\left(\frac{1}{\sqrt{8}}\right) - \frac{4}{15}G$ $+\frac{4}{5}\text{Ti}_2(3 - 2\sqrt{2})$
4	any	Formula (55), using known $B_n$ -residues as needed

TABLE 8. Example evaluations of  $\Delta_5(s)$ . It is proven that every  $\Delta_5(\text{odd})$  is hyperclosed. Every  $\Delta_5(\text{even})$  is hyperclosed, with perhaps three exceptions as in the table.

$n$	$s$	$\Delta_n(s)$
5	$-5, \dots, -10$	$\infty$
5	1	$-\frac{1279}{567}G - \frac{4}{189}\pi + \frac{4}{315}\pi^2 - \frac{449}{3465} + \frac{3239}{62370}\sqrt{2} + \frac{568}{3465}\sqrt{3} - \frac{380}{6237}\sqrt{5}$ $+\frac{295}{252}\log 3 + \frac{1}{54}\log(1 + \sqrt{2}) + \frac{20}{63}\log(2 + \sqrt{3}) + \frac{64}{189}\log\left(\frac{1+\sqrt{5}}{2}\right)$ $-\frac{73}{63}\sqrt{2} \arctan\left(\frac{1}{\sqrt{8}}\right) - \frac{8}{21}\sqrt{3} \arctan\left(\frac{1}{\sqrt{15}}\right) + \frac{104}{63}\log(2 - \sqrt{3})\theta$ $+\frac{5}{7}\text{Ti}_2(3 - 2\sqrt{2}) + \frac{104}{63}\text{Cl}_2\left(\frac{1}{3}\theta + \frac{1}{3}\pi\right) - \frac{104}{63}\text{Cl}_2\left(\frac{1}{3}\theta - \frac{1}{6}\pi\right)$ $-\frac{104}{189}\text{Cl}_2\left(\theta + \frac{1}{6}\pi\right) - \frac{208}{189}\text{Cl}_2\left(\theta + \frac{4}{3}\pi\right) + \frac{104}{189}\text{Cl}_2\left(\theta + \frac{5}{3}\pi\right) + \frac{208}{189}\text{Cl}_2\left(\theta + \frac{11}{6}\pi\right)$
5	any odd	Closed forms follow from (56), using residues as needed
5	any even	Closed forms follow from (56), using residues as needed, with only $\Delta_5(-2), \Delta_5(-4), \Delta(-12)$ remaining unresolved.

## 12. CONJECTURES AND OPEN QUESTIONS

We conclude by reiterating the following open questions.

- (1) Is it a reasonable conjecture that *every* box integral  $B_{\text{integer}}(\text{integer})$ ,  $\Delta_{\text{integer}}(\text{integer})$  be hyperclosed? That is, could it be that our results for  $n \leq 4$  are actually extensible for all positive integer  $n$ ?
- (2) Is there a general evaluation (hyperclosed or not) of  $B_n(-n-1)$  for all natural numbers  $n$ ?
- (3) What transpires for noninteger but rational  $s$  in dimension  $n \leq 5$  (see relation (72))?
- (4) Can  $\mathcal{K}_5$  be resolved? As we have said, this is the sole blockade to proof of hyperclosure for all  $B_5(\text{integer})$ ,  $\Delta_5(\text{integer})$ .
- (5) Referring to Figure 1, what is a closed form for the mysterious zero? Are there any other (possibly complex) zeros of any  $\Delta_n$  whatsoever? Is there a closed form for the local minimum of  $B_2(s)$  at  $s \approx 3.667\dots$ ?
- (6) What is an explicit number that is not hyperclosed? Even though almost all numbers are not hyperclosed, we presently do not know of a single such number. We have suggested that perhaps  $\pi^\pi$  is not hyperclosed; moreover, in the absence of known hypergeometric forms for the Euler constant  $\gamma$ , one is tempted to conjecture that it, too, is not hyperclosed.

## 13. APPENDIX: COMPENDIUM OF PROVEN CLOSED FORMS

Numerical tables in support of the following closed forms are to be found at <http://crd.lbl.gov/~dhbailey/dhbpapers/box-int-b-delta.txt>

## ACKNOWLEDGMENTS

The authors are grateful to T. Wieting for clarifications on hypergeometric algebra, as well as to O-Y. Chan, G. Lamb, J. Philip, M. Trott, and E. Weisstein for their contributions to box-integral theory. In particular, the Clausen terms in earlier formulae for  $\Delta_4(1)$ ,  $\Delta_5(1)$  in [5] needed repair; we thank J. Philip for pointing this out in his delightful paper [21].<sup>9</sup> Finally, the authors are deeply indebted to A. Kaiser of U.C. Berkeley and LBNL for writing computer code to check the formulae presented in the Appendix.

## REFERENCES

- [1] R. Anderssen, R. Brent, D. Daley, and P. Moran, "Concerning  $\int_0^1 \dots \int_0^1 (x_1^2 + \dots + x_n^2)^{\frac{1}{2}} dx_1 \dots dx_n$  and a Taylor series method," *SIAM J. Applied Math.*, **30** (1976), 22–30. MR0394974 (52:15773)
- [2] M. Abramowitz and I.A. Stegun, *Handbook of Mathematical Functions*, NBS (now NIST), 1965. See also <http://dlmf.nist.gov/>.
- [3] David H. Bailey and Jonathan M. Borwein, "Highly parallel, high-precision numerical integration," *Int. Journal of Computational Science and Engineering*, accepted Jan. 2008. Available at <http://crd.lbl.gov/~dhbailey/dhbpapers/quadparallel.pdf>.
- [4] David H. Bailey and Jonathan M. Borwein, "Effective error bounds for Euler-Maclaurin-based quadrature schemes," *20th Annual HPCS Proceedings*, IEEE CD, May 2006. Available at <http://crd.lbl.gov/~dhbailey/dhbpapers/em-error.pdf>.

<sup>9</sup>Therein his formula for  $\Delta_4(1)$  has yet a newer misprint. As mentioned in Section 4, the present authors believe that the best way to ascertain what version of a recondite closed form be the correct one across publications, say—is to test expressions via extreme numerical precision.

- [5] D.H. Bailey, J.M. Borwein and R.E. Crandall, "Box integrals," *Journal of Computational and Applied Mathematics*, **206** (2007), 196–208. [D-drive Preprint 320]. MR2337437 (2008i:65036)
- [6] D.H. Bailey, J.M. Borwein and R.E. Crandall, "Integrals of the Ising class," *J. Phys. A.*, **39** (2006), 12271–12302. Available at <http://crd.lbl.gov/~dhbailey/dhbpapers/Ising.pdf>. MR2261886 (2007j:33044)
- [7] David H. Bailey, Jonathan M. Borwein, Vishaal Kapoor, and Eric W. Weisstein, "Ten problems in experimental mathematics," *Amer. Mathematical Monthly*, **113** (2006), 481–509. Available at <http://locutus.cs.dal.ca:8088/archive/00000316/> MR2231135 (2007b:65001)
- [8] David H. Bailey and David J. Broadhurst, "Parallel integer relation detection: Techniques and applications," *Mathematics of Computation*, **70** (Oct 2000), 1719–1736. MR1836930 (2002b:11174)
- [9] David H. Bailey, Xiaoye S. Li and Karthik Jeyabalan, "A comparison of three high-precision quadrature schemes," *Experimental Mathematics*, **14** (2005), 317–329. Available at <http://crd.lbl.gov/~dhbailey/dhbpapers/quadrature.pdf>. MR2172710 (2006e:65047)
- [10] David H. Bailey, Yozo Hida, Xiaoye S. Li and Brandon Thompson, "ARPREC: An arbitrary precision computation package," September 2002. Available at <http://crd.lbl.gov/~dhbailey/dhbpapers/arprec.pdf>.
- [11] Jonathan M. Borwein and David H. Bailey, *Mathematics by Experiment*, AK Peters, 2003. Second edition, 2008. See also <http://www.experimentalmath.info>. MR2473161 (2010c:00001)
- [12] J. M. Borwein and B. Salvy, "A proof of a recursion for Bessel moments," *Exp. Mathematics*, vol. 17 (2008), 223–230. MR2433887
- [13] Chaunming Zong, *The Cube-A Window to Convex and Discrete Geometry*, Cambridge Tracts in Mathematics, 2006.
- [14] R.E. Crandall, C. Joe, and T. Mehoke, "On the fractal distribution of brain synapses," manuscript, 2009.
- [15] Helaman R. P. Ferguson, David H. Bailey and Stephen Arno, "Analysis of PSLQ, an integer relation finding algorithm," *Mathematics of Computation*, **68** (Jan 1999), 351–369. MR1489971 (99c:11157)
- [16] Wolfram Koepf, *Hypergeometric Summation: An Algorithmic Approach to Summation and Special Function Identities*, American Mathematical Society, Providence, RI, 1998. MR1644447 (2000c:33002)
- [17] G. Lamb, "An evaluation of the integral  $\mathcal{K}_0$ ," "A method of evaluating the integral  $\mathcal{K}_1$ ," and "An approach to evaluating the integral  $\mathcal{K}_3$ ," preprint collection, 2006.
- [18] G. Lamb, "An evaluation of the integral  $\mathcal{K}_6$ ," and "An approach to evaluating the integral  $\mathcal{K}_4$ ," preprint collection, 2009.
- [19] Leonard Lewin, *Polylogarithms and Associated Functions*, North Holland, 1981. MR618278 (83b:33019)
- [20] Jack Dongarra, Jim Bunch, Cleve Moler, Pete Stewart, *LINPACK User's Guide*, SIAM, Philadelphia, 1979.
- [21] J. Philip, "The distance between two random points in a 4- and 5-cube," preprint, 2008.
- [22] D. Robbins, "Average distance between two points in a box," *Amer. Mathematical Monthly*, **85** (1978), 278.
- [23] Charles Schwartz, "Numerical integration of analytic functions," *Journal of Computational Physics*, **4** (1969), 19–29. MR0243741 (39:5062)
- [24] Hidetosi Takahasi and Masatake Mori, "Quadrature formulas obtained by variable transformation," *Numerische Mathematik*, **21** (1973), 206–219. MR0331738 (48:10070)
- [25] M. Trott, Private communication, 2005.
- [26] M. Trott, "The area of a random triangle," *Mathematica Journal*, **7** (1998), 189–198.
- [27] E. Weisstein, "Hypercube line picking." Available at <http://mathworld.wolfram.com/HypercubeLinePicking.html>.

LAWRENCE BERKELEY NATIONAL LABORATORY, BERKELEY, CALIFORNIA 94720

*E-mail address:* `dhbailey@lbl.gov`

SCHOOL OF MATHEMATICAL AND PHYSICAL SCIENCES, UNIVERSITY OF NEWCASTLE, CALLAGHAN,  
NSW 2308, AUSTRALIA AND FACULTY OF COMPUTER SCIENCE, DALHOUSIE UNIVERSITY, HALIFAX,  
NS, B3H 2W5, CANADA

*E-mail address:* `jonathan.borwein@newcastle.edu.au`

*E-mail address:* `jborwein@cs.dal.ca`

CENTER FOR ADVANCED COMPUTATION, REED COLLEGE, PORTLAND, OREGON

*E-mail address:* `crandall@reed.edu`